

Tris(2-butoxyethyl) phosphate  
78-51-3 | DTXSID5021758

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:**  $1.73\text{e-}11$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Outside

**Local applicability domain index:**  $2.14\text{e-}01$

**Confidence level:**  $7.81\text{e-}01$

## Nearest Neighbors from the Training Set

Image not found

Isoproturon

**Measured:**  $1.20\text{e-}11$

**Predicted:**  $3.23\text{e-}11$

Image not found

Terbutylazine

**Measured:**  $1.10\text{e-}11$

**Predicted:**  $1.23\text{e-}11$

Image not found

Cycloate

**Measured:**  $3.54\text{e-}11$

**Predicted:**  $2.98\text{e-}11$

Image not found

Bornyl acetate

**Measured:**  $1.39\text{e-}11$

**Predicted:**  $1.36\text{e-}11$

Image not found

4,4'-Methylenedianiline

**Measured:**  $3.00\text{e-}11$

**Predicted:**  $4.28\text{e-}11$